



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2023 – 10:10 PM EDT

PDB ID : 2HNE  
Title : Crystal structure of l-fuconate dehydratase from xanthomonas campestris pv. campestris str. ATCC 33913  
Authors : Fedorov, A.A.; Fedorov, E.V.; Yew, W.S.; Gerlt, J.A.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2006-07-12  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

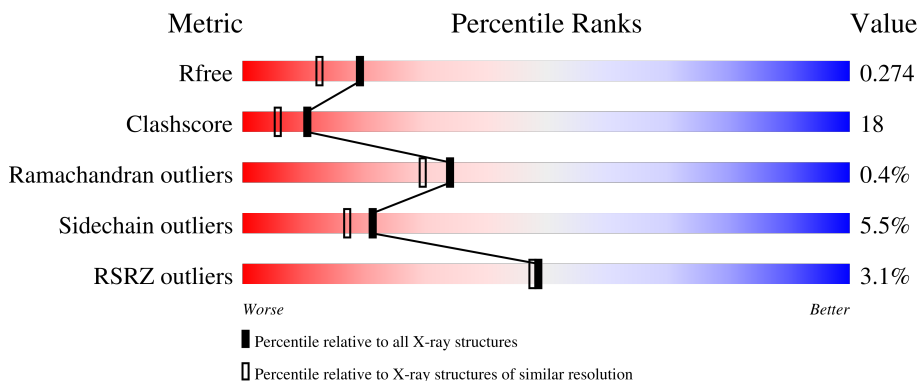
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	436	
1	B	436	
1	C	436	
1	D	436	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13619 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called L-fuconate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	426	Total 3295	C 2091	N 587	O 607	S 10	0	0	0
1	B	432	Total 3334	C 2112	N 594	O 617	S 11	0	0	0
1	C	434	Total 3350	C 2122	N 596	O 621	S 11	0	0	0
1	D	433	Total 3341	C 2116	N 595	O 619	S 11	0	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0
2	B	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0
2	D	1	Total 1	Mg 1	0	0

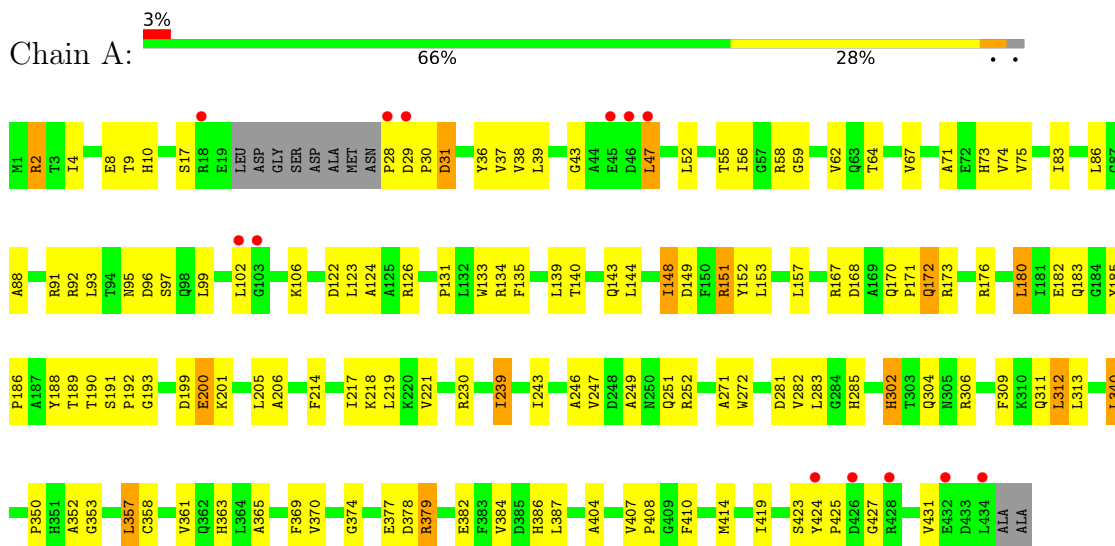
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	76	Total 76	O 76	0	0
3	B	91	Total 91	O 91	0	0
3	C	63	Total 63	O 63	0	0
3	D	65	Total 65	O 65	0	0

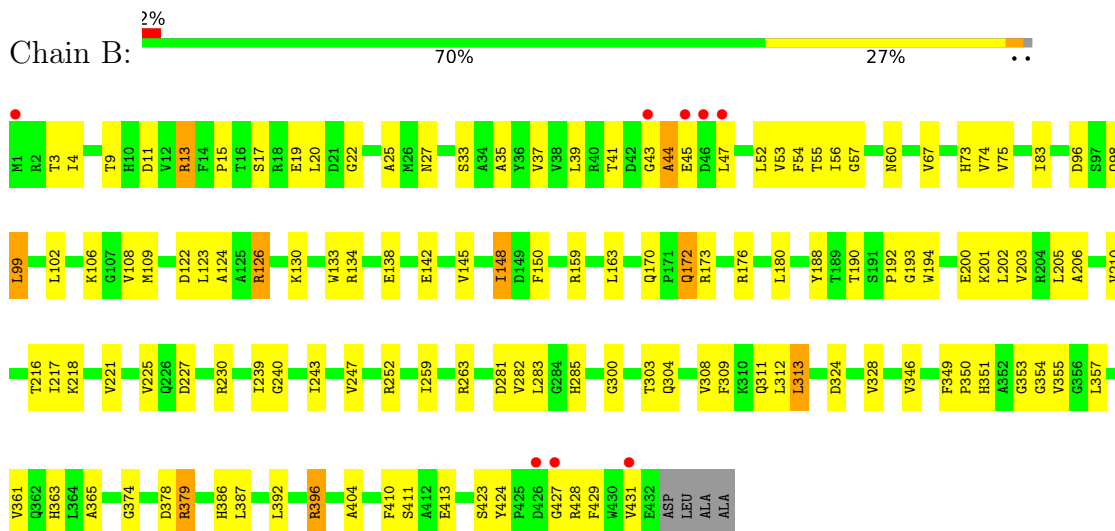
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: L-fuconate dehydratase



- Molecule 1: L-fuconate dehydratase



- Molecule 1: L-fuconate dehydratase





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.63Å 130.63Å 195.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.68 – 2.00 39.19 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.1 (24.68-2.00) 91.8 (39.19-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 1.89Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.241 , 0.274 0.241 , 0.274	Depositor DCC
$R_{free}$ test set	7677 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.1	Xtrriage
Anisotropy	0.027	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13619	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.33	0/3367	0.63	0/4584
1	B	0.36	0/3407	0.67	1/4640 (0.0%)
1	C	0.32	0/3423	0.62	0/4662
1	D	0.33	0/3413	0.63	1/4646 (0.0%)
All	All	0.34	0/13610	0.64	2/18532 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	193	GLY	N-CA-C	5.37	126.52	113.10
1	D	35	ALA	N-CA-C	-5.03	97.42	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3295	0	3265	122	0
1	B	3334	0	3297	129	0
1	C	3350	0	3312	158	0
1	D	3341	0	3303	115	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	76	0	0	1	0
3	B	91	0	0	2	0
3	C	63	0	0	2	0
3	D	65	0	0	5	0
All	All	13619	0	13177	487	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (487) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:VAL:HG11	1:B:67:VAL:HG11	1.22	1.08
1:B:239:ILE:HG23	1:B:243:ILE:HB	1.39	1.05
1:D:170:GLN:HA	1:D:173:ARG:HD3	1.41	1.02
1:A:122:ASP:O	1:A:126:ARG:HG2	1.61	1.01
1:B:170:GLN:HA	1:B:173:ARG:HD3	1.44	1.00
1:C:239:ILE:HG23	1:C:243:ILE:HB	1.44	0.97
1:C:170:GLN:HA	1:C:173:ARG:HD3	1.52	0.90
1:C:134:ARG:O	1:C:138:GLU:HG2	1.73	0.88
1:B:122:ASP:O	1:B:126:ARG:HG2	1.74	0.86
1:B:9:THR:HG22	1:B:37:VAL:HG12	1.56	0.85
1:D:198:SER:HB3	1:D:201:LYS:HB2	1.57	0.85
1:B:239:ILE:CG2	1:B:243:ILE:HB	2.08	0.84
1:C:239:ILE:CG2	1:C:243:ILE:HB	2.08	0.82
1:D:11:ASP:OD1	1:D:13:ARG:HD3	1.80	0.82
1:B:206:ALA:HB1	1:B:239:ILE:CD1	2.12	0.79
1:D:192:PRO:HB2	1:D:217:ILE:HD11	1.67	0.77
1:A:151:ARG:HD3	1:A:152:TYR:CE2	2.19	0.77
1:C:133:TRP:H	1:C:363:HIS:HD2	1.35	0.75
1:D:151:ARG:HD3	1:D:152:TYR:CE2	2.21	0.74
1:D:55:THR:HG23	3:D:605:HOH:O	1.88	0.74
1:C:247:VAL:HG12	1:C:273:ILE:HD13	1.70	0.73
1:B:13:ARG:HB3	1:B:33:SER:OG	1.89	0.73
1:B:192:PRO:HB2	1:B:217:ILE:HD11	1.70	0.72
1:A:171:PRO:HB2	1:A:172:GLN:OE1	1.89	0.72
1:A:283:LEU:H	1:B:311:GLN:HE21	1.38	0.72
1:A:170:GLN:HB3	1:A:171:PRO:HD3	1.69	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:ARG:HD3	1:C:152:TYR:CE2	2.25	0.71
1:C:387:LEU:HA	1:C:389:GLN:HE22	1.55	0.70
1:A:83:ILE:HD11	1:A:123:LEU:HD22	1.72	0.70
1:C:378:ASP:OD1	1:C:379:ARG:HD2	1.92	0.70
1:D:239:ILE:HG23	1:D:243:ILE:HB	1.74	0.69
3:A:603:HOH:O	1:B:55:THR:HG23	1.90	0.69
1:A:58:ARG:HG3	1:B:98:GLN:OE1	1.92	0.69
1:C:282:VAL:H	1:D:311:GLN:HE22	1.39	0.69
1:B:145:VAL:HG11	1:B:159:ARG:HG3	1.74	0.68
1:B:142:GLU:HG2	1:D:200:GLU:HG2	1.75	0.68
1:D:324:ASP:OD2	1:D:351:HIS:HD2	1.75	0.68
1:B:37:VAL:CG1	1:B:67:VAL:HG11	2.12	0.68
1:A:180:LEU:HD22	1:A:404:ALA:HB2	1.75	0.67
1:A:10:HIS:HB2	1:A:36:TYR:HB3	1.75	0.67
1:A:2:ARG:HB2	1:A:2:ARG:NH2	2.09	0.67
1:D:192:PRO:CB	1:D:217:ILE:HD11	2.25	0.66
1:B:225:VAL:HG23	3:B:657:HOH:O	1.94	0.66
1:A:239:ILE:HG23	1:A:243:ILE:HB	1.78	0.66
1:A:378:ASP:OD1	1:A:379:ARG:HD2	1.96	0.66
1:A:28:PRO:C	1:A:30:PRO:HD3	2.16	0.66
1:A:58:ARG:NH1	1:B:98:GLN:HG3	2.11	0.66
1:D:172:GLN:H	1:D:172:GLN:NE2	1.92	0.66
1:A:427:GLY:O	1:A:431:VAL:HG23	1.96	0.66
1:C:328:VAL:HG22	1:C:333:GLU:OE2	1.95	0.66
1:B:133:TRP:H	1:B:363:HIS:HD2	1.42	0.65
1:C:122:ASP:O	1:C:126:ARG:HG2	1.96	0.65
1:D:47:LEU:HD13	1:D:123:LEU:HD21	1.76	0.65
1:D:206:ALA:HB1	1:D:239:ILE:HD13	1.79	0.65
1:C:13:ARG:HG3	1:C:424:TYR:HB2	1.78	0.65
1:B:15:PRO:HG3	1:B:429:PHE:CZ	2.31	0.65
1:D:52:LEU:CD2	1:D:360:LEU:HD11	2.27	0.65
1:D:52:LEU:HD21	1:D:360:LEU:HD11	1.79	0.65
1:C:133:TRP:H	1:C:363:HIS:CD2	2.15	0.65
1:D:13:ARG:HG3	1:D:424:TYR:HB2	1.79	0.65
1:B:239:ILE:HG22	1:B:240:GLY:O	1.97	0.65
1:C:170:GLN:HA	1:C:173:ARG:CD	2.26	0.64
1:B:172:GLN:H	1:B:172:GLN:HE21	1.44	0.64
1:C:54:PHE:HB2	1:C:357:LEU:HD21	1.78	0.64
1:D:2:ARG:HG3	1:D:79:VAL:HB	1.79	0.64
1:D:172:GLN:NE2	1:D:172:GLN:N	2.46	0.64
1:C:328:VAL:HG22	1:C:329:GLY:H	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:GLY:O	1:C:62:VAL:HG22	1.98	0.64
1:C:225:VAL:HG23	3:C:653:HOH:O	1.96	0.64
1:D:83:ILE:HD12	1:D:124:ALA:CA	2.28	0.64
1:B:180:LEU:CD2	1:B:404:ALA:HB2	2.27	0.63
1:B:259:ILE:O	1:B:263:ARG:HG3	1.98	0.63
1:D:83:ILE:HD12	1:D:124:ALA:HA	1.80	0.63
1:B:145:VAL:CG1	1:B:159:ARG:HG3	2.28	0.63
1:C:2:ARG:NH2	1:C:47:LEU:HD11	2.14	0.63
1:A:133:TRP:H	1:A:363:HIS:HD2	1.45	0.63
1:B:201:LYS:O	1:B:205:LEU:HD13	1.99	0.63
1:A:414:MET:HB2	1:A:419:ILE:HD11	1.81	0.63
1:C:131:PRO:HG2	1:C:134:ARG:HB2	1.80	0.63
1:B:130:LYS:HE3	1:B:138:GLU:OE2	1.98	0.62
1:C:206:ALA:HB1	1:C:239:ILE:CD1	2.29	0.62
1:A:283:LEU:H	1:B:311:GLN:NE2	1.96	0.62
1:A:282:VAL:H	1:B:311:GLN:HE22	1.47	0.62
1:C:37:VAL:HG22	1:C:67:VAL:HG11	1.81	0.62
1:C:386:HIS:HB3	1:C:387:LEU:HD22	1.81	0.62
1:B:148:ILE:HG12	1:B:150:PHE:CE1	2.34	0.62
1:A:88:ALA:O	1:A:92:ARG:HG3	2.00	0.62
1:A:309:PHE:O	1:A:313:LEU:HD13	2.00	0.61
1:D:8:GLU:HB2	1:D:38:VAL:HB	1.82	0.61
1:A:59:GLY:O	1:A:62:VAL:HG22	2.00	0.61
1:A:168:ASP:O	1:A:171:PRO:HD2	2.00	0.61
1:B:227:ASP:OD2	1:B:230:ARG:NH1	2.34	0.61
1:B:428:ARG:O	1:B:431:VAL:HG12	2.00	0.61
1:C:311:GLN:HE22	1:D:282:VAL:H	1.48	0.61
1:D:133:TRP:H	1:D:363:HIS:HD2	1.46	0.61
1:A:206:ALA:HB1	1:A:239:ILE:HD13	1.82	0.60
1:D:433:ASP:C	1:D:435:ALA:H	2.04	0.60
1:C:283:LEU:H	1:D:311:GLN:HE21	1.49	0.60
1:A:311:GLN:HE22	1:B:282:VAL:H	1.50	0.60
1:B:180:LEU:HD22	1:B:404:ALA:HB2	1.84	0.60
1:C:37:VAL:CG2	1:C:67:VAL:HG11	2.32	0.60
1:D:353:GLY:O	1:D:357:LEU:HB2	2.02	0.60
1:A:193:GLY:HA3	1:A:219:LEU:HA	1.84	0.59
1:B:396:ARG:HG2	1:B:396:ARG:HH11	1.67	0.59
1:C:262:MET:HA	1:C:262:MET:HE2	1.85	0.59
1:B:55:THR:HG22	1:B:57:GLY:H	1.67	0.59
1:C:311:GLN:HE21	1:D:283:LEU:H	1.50	0.58
1:C:282:VAL:N	1:D:311:GLN:HE22	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:VAL:O	1:D:207:LYS:HD3	2.03	0.58
1:A:282:VAL:N	1:B:311:GLN:HE22	2.01	0.58
1:C:360:LEU:HD21	1:C:412:ALA:HB2	1.86	0.58
1:B:313:LEU:HD11	1:B:346:VAL:HG21	1.85	0.58
1:D:207:LYS:HG3	1:D:238:ALA:HB1	1.86	0.58
1:C:201:LYS:HG2	1:C:205:LEU:HD23	1.86	0.57
1:C:130:LYS:NZ	1:C:138:GLU:HG3	2.19	0.57
1:C:407:VAL:HG13	1:C:408:PRO:HD2	1.85	0.57
1:A:131:PRO:HG2	1:A:134:ARG:HB2	1.87	0.57
1:C:145:VAL:O	1:C:148:ILE:HG23	2.05	0.57
1:A:37:VAL:HG22	1:A:67:VAL:HG11	1.86	0.57
1:A:170:GLN:HA	1:A:173:ARG:HD3	1.87	0.57
1:D:73:HIS:HE1	1:D:96:ASP:OD2	1.87	0.57
1:C:262:MET:CE	1:C:265:LEU:HD12	2.35	0.57
1:C:62:VAL:HG21	1:D:109:MET:CE	2.35	0.57
1:D:363:HIS:HE1	1:D:411:SER:OG	1.88	0.56
1:D:200:GLU:O	1:D:203:VAL:HG22	2.05	0.56
1:B:55:THR:HG21	1:B:60:ASN:HB2	1.87	0.56
1:C:55:THR:HG23	3:D:644:HOH:O	2.03	0.56
1:D:387:LEU:N	1:D:387:LEU:HD12	2.20	0.56
1:A:200:GLU:OE1	1:C:159:ARG:NH1	2.39	0.56
1:D:360:LEU:HD21	1:D:412:ALA:HB2	1.87	0.56
1:B:35:ALA:HB3	1:B:53:VAL:HB	1.88	0.56
1:C:180:LEU:CD2	1:C:404:ALA:HB2	2.34	0.56
1:C:180:LEU:HD22	1:C:404:ALA:HB2	1.86	0.56
1:C:71:ALA:O	1:C:75:VAL:HG22	2.04	0.56
1:C:387:LEU:HA	1:C:389:GLN:NE2	2.20	0.56
1:B:428:ARG:HG2	1:B:428:ARG:HH11	1.70	0.56
1:B:172:GLN:H	1:B:172:GLN:NE2	2.04	0.56
1:A:17:SER:HB2	1:A:31:ASP:OD1	2.06	0.55
1:A:419:ILE:O	1:A:423:SER:HB2	2.06	0.55
1:C:204:ARG:O	1:C:208:GLU:HG3	2.06	0.55
1:D:172:GLN:H	1:D:172:GLN:HE21	1.53	0.55
1:D:386:HIS:HB3	1:D:387:LEU:HD13	1.88	0.55
1:B:148:ILE:HD11	1:B:150:PHE:CE2	2.41	0.55
1:D:207:LYS:HZ2	1:D:207:LYS:HB2	1.72	0.55
1:D:201:LYS:O	1:D:201:LYS:HD3	2.06	0.55
1:C:368:ASP:OD2	1:C:372:ILE:HB	2.07	0.54
1:C:375:LYS:O	1:C:379:ARG:HD3	2.08	0.54
1:B:363:HIS:HE1	1:B:411:SER:OG	1.89	0.54
1:A:52:LEU:HD12	1:A:52:LEU:C	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:GLU:HB2	3:C:648:HOH:O	2.07	0.54
1:C:350:PRO:HB3	1:C:361:VAL:HG21	1.89	0.54
1:A:407:VAL:HG13	1:A:408:PRO:HD2	1.89	0.54
1:C:79:VAL:O	1:C:83:ILE:HD13	2.08	0.54
1:C:70:LEU:HD12	1:C:116:VAL:HG21	1.89	0.54
1:B:324:ASP:OD2	1:B:351:HIS:HD2	1.91	0.54
1:A:172:GLN:O	1:A:176:ARG:HG3	2.08	0.54
1:C:189:THR:HG23	1:C:217:ILE:CD1	2.37	0.53
1:D:201:LYS:O	1:D:205:LEU:HD13	2.09	0.53
1:C:15:PRO:HG3	1:C:429:PHE:CZ	2.43	0.53
1:C:262:MET:HA	1:C:262:MET:CE	2.39	0.53
1:D:37:VAL:HG22	1:D:67:VAL:HG11	1.90	0.53
1:B:378:ASP:OD1	1:B:379:ARG:HD2	2.08	0.53
1:C:145:VAL:HG13	1:C:150:PHE:CZ	2.44	0.53
1:C:239:ILE:HG22	1:C:240:GLY:O	2.08	0.53
1:B:180:LEU:O	1:B:180:LEU:HD23	2.09	0.53
1:B:387:LEU:N	1:B:387:LEU:HD12	2.24	0.53
1:C:20:LEU:N	1:C:20:LEU:HD12	2.24	0.53
1:D:206:ALA:HB1	1:D:239:ILE:CD1	2.38	0.53
1:B:145:VAL:HG13	1:B:150:PHE:CZ	2.43	0.53
1:A:8:GLU:CG	1:A:38:VAL:HB	2.39	0.53
1:A:139:LEU:HB2	1:A:144:LEU:HD13	1.91	0.53
1:C:189:THR:HG23	1:C:217:ILE:HD12	1.91	0.53
1:A:387:LEU:N	1:A:387:LEU:HD22	2.24	0.53
1:D:419:ILE:O	1:D:423:SER:HB2	2.09	0.52
1:C:221:VAL:CG2	1:C:247:VAL:HG13	2.40	0.52
1:C:384:VAL:HG12	1:C:386:HIS:ND1	2.25	0.52
1:A:249:ALA:O	1:A:252:ARG:HG3	2.09	0.52
1:A:62:VAL:HG21	1:B:109:MET:CE	2.40	0.52
1:C:83:ILE:HG13	1:C:124:ALA:HA	1.90	0.52
1:C:311:GLN:NE2	1:D:283:LEU:H	2.07	0.52
1:A:206:ALA:HB1	1:A:239:ILE:CD1	2.40	0.52
1:B:206:ALA:HB1	1:B:239:ILE:HD11	1.90	0.52
1:B:392:LEU:HD13	1:B:413:GLU:HG2	1.92	0.52
1:A:353:GLY:O	1:A:357:LEU:HB2	2.09	0.52
1:A:423:SER:O	1:A:427:GLY:HA3	2.10	0.52
1:C:145:VAL:HG21	1:C:163:LEU:HG	1.92	0.52
1:B:357:LEU:N	1:B:357:LEU:HD22	2.25	0.52
1:B:386:HIS:HB3	1:B:387:LEU:HD13	1.92	0.52
1:C:109:MET:HE1	1:D:62:VAL:HG11	1.91	0.52
1:C:349:PHE:CZ	1:C:379:ARG:HA	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:GLN:NE2	1:B:172:GLN:N	2.58	0.52
1:B:349:PHE:CZ	1:B:379:ARG:HA	2.44	0.52
1:A:83:ILE:CD1	1:A:123:LEU:HD22	2.40	0.52
1:A:55:THR:HG22	1:A:56:ILE:N	2.25	0.51
1:D:207:LYS:HB2	1:D:207:LYS:NZ	2.24	0.51
1:A:369:PHE:O	1:A:374:GLY:HA2	2.09	0.51
1:D:267:GLU:C	1:D:269:ASP:H	2.13	0.51
1:C:15:PRO:O	1:C:18:ARG:HG2	2.11	0.51
1:C:55:THR:HG22	1:C:57:GLY:H	1.75	0.51
1:C:56:ILE:HG13	1:D:98:GLN:HG2	1.91	0.51
1:C:311:GLN:HE22	1:D:282:VAL:N	2.08	0.51
1:C:226:GLN:H	1:C:226:GLN:NE2	2.08	0.51
1:B:54:PHE:HB2	1:B:357:LEU:HD21	1.92	0.51
1:C:206:ALA:HB1	1:C:239:ILE:HD13	1.93	0.51
1:C:172:GLN:NE2	1:C:172:GLN:H	2.08	0.51
1:D:267:GLU:HG3	1:D:268:PHE:N	2.26	0.51
1:A:239:ILE:CG2	1:A:243:ILE:HB	2.39	0.51
1:B:221:VAL:HG22	1:B:247:VAL:HG13	1.93	0.51
1:C:139:LEU:HB2	1:C:144:LEU:HD21	1.93	0.51
1:B:17:SER:HA	3:B:649:HOH:O	2.11	0.50
1:C:283:LEU:H	1:D:311:GLN:NE2	2.09	0.50
1:C:52:LEU:N	1:C:52:LEU:HD23	2.26	0.50
1:A:102:LEU:HD12	1:B:108:VAL:HG22	1.93	0.50
1:A:191:SER:OG	1:A:192:PRO:HD3	2.11	0.50
1:D:251:GLN:HE22	1:D:302:HIS:CD2	2.29	0.50
1:B:176:ARG:CD	1:B:374:GLY:HA2	2.41	0.50
1:B:221:VAL:CG2	1:B:247:VAL:CG1	2.89	0.50
1:C:105:GLU:HA	1:C:110:HIS:ND1	2.26	0.50
1:D:173:ARG:HD2	3:D:626:HOH:O	2.11	0.50
1:B:22:GLY:HA2	1:B:194:TRP:CZ3	2.46	0.50
1:B:221:VAL:CG2	1:B:247:VAL:HG13	2.42	0.50
1:B:45:GLU:C	1:B:47:LEU:H	2.15	0.50
1:D:83:ILE:HD11	1:D:123:LEU:HD13	1.93	0.50
1:D:202:LEU:HD12	1:D:202:LEU:C	2.32	0.49
1:C:192:PRO:HB3	1:C:205:LEU:HB3	1.94	0.49
1:B:188:TYR:HB2	1:B:216:THR:HB	1.94	0.49
1:C:302:HIS:HD2	1:D:104:PRO:HD3	1.78	0.49
1:C:192:PRO:O	1:C:202:LEU:HD23	2.12	0.49
1:A:182:GLU:HG3	1:A:183:GLN:N	2.28	0.49
1:C:376:MET:HA	1:C:379:ARG:HD3	1.93	0.49
1:A:189:THR:HG23	1:A:214:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:GLN:HE21	1:B:172:GLN:N	2.10	0.49
1:C:389:GLN:CD	1:C:389:GLN:H	2.15	0.49
1:D:159:ARG:HG3	1:D:160:ASP:N	2.28	0.49
1:B:19:GLU:O	1:B:20:LEU:HB2	2.13	0.49
1:B:43:GLY:O	1:B:44:ALA:C	2.51	0.49
1:C:83:ILE:HD11	1:C:123:LEU:HD22	1.95	0.49
1:C:104:PRO:HD3	1:D:302:HIS:HD2	1.78	0.49
1:A:2:ARG:HB2	1:A:2:ARG:HH21	1.76	0.48
1:B:25:ALA:HB1	1:B:252:ARG:HG3	1.94	0.48
1:A:176:ARG:HD2	1:A:370:VAL:O	2.13	0.48
1:B:221:VAL:HG21	1:B:247:VAL:CG1	2.42	0.48
1:C:247:VAL:HG12	1:C:273:ILE:CD1	2.40	0.48
1:D:135:PHE:O	1:D:139:LEU:HG	2.13	0.48
1:B:45:GLU:HA	1:B:45:GLU:OE2	2.13	0.48
1:C:24:ASP:HB2	1:C:250:ASN:ND2	2.28	0.48
1:C:55:THR:CG2	1:C:56:ILE:N	2.77	0.48
1:C:73:HIS:HE1	1:C:96:ASP:OD2	1.96	0.48
1:C:236:ARG:HH21	1:C:269:ASP:HB3	1.78	0.48
1:C:22:GLY:HA2	1:C:194:TRP:CZ3	2.49	0.48
1:C:148:ILE:HG13	1:C:149:ASP:N	2.27	0.48
1:C:151:ARG:HD3	1:C:152:TYR:CZ	2.48	0.48
1:C:350:PRO:HB3	1:C:361:VAL:CG2	2.44	0.48
1:C:369:PHE:O	1:C:374:GLY:HA2	2.14	0.48
1:C:428:ARG:HG2	1:C:428:ARG:HH11	1.76	0.48
1:A:199:ASP:OD2	1:A:230:ARG:NH2	2.47	0.48
1:B:83:ILE:HG23	1:B:124:ALA:CB	2.43	0.48
1:C:8:GLU:HB2	1:C:38:VAL:HB	1.94	0.48
1:B:355:VAL:O	1:B:357:LEU:HD22	2.14	0.48
1:C:13:ARG:HG3	1:C:424:TYR:CB	2.43	0.48
1:B:200:GLU:O	1:B:203:VAL:HG22	2.13	0.48
1:A:92:ARG:HB3	1:A:92:ARG:NH2	2.28	0.48
1:B:73:HIS:HE1	1:B:96:ASP:OD2	1.96	0.48
1:D:369:PHE:CD2	1:D:376:MET:HB3	2.49	0.48
1:A:83:ILE:HG13	1:A:124:ALA:HA	1.96	0.48
1:D:204:ARG:HA	1:D:207:LYS:HZ2	1.78	0.48
1:D:387:LEU:N	1:D:387:LEU:CD1	2.77	0.47
1:C:139:LEU:HB2	1:C:144:LEU:CD2	2.45	0.47
1:C:176:ARG:HD3	1:C:374:GLY:HA2	1.94	0.47
1:C:130:LYS:HZ3	1:C:138:GLU:HG3	1.78	0.47
1:A:311:GLN:NE2	1:B:283:LEU:H	2.12	0.47
1:A:350:PRO:HG2	1:A:365:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:LEU:HD12	1:D:203:VAL:N	2.29	0.47
1:A:281:ASP:O	1:A:285:HIS:HD2	1.97	0.47
1:A:91:ARG:O	1:A:95:ASN:HB2	2.14	0.47
1:A:139:LEU:HD12	1:A:144:LEU:CD1	2.45	0.47
1:B:428:ARG:HG2	1:B:428:ARG:NH1	2.29	0.47
1:C:2:ARG:HH21	1:C:47:LEU:HD11	1.78	0.47
1:C:180:LEU:HD23	1:C:180:LEU:O	2.15	0.47
1:A:190:THR:HG21	1:A:382:GLU:OE2	2.15	0.47
1:A:47:LEU:HD11	1:A:123:LEU:HD21	1.97	0.47
1:B:308:VAL:O	1:B:312:LEU:CD2	2.63	0.47
1:D:207:LYS:CD	1:D:238:ALA:HB1	2.45	0.47
1:D:378:ASP:OD1	1:D:379:ARG:CD	2.63	0.47
1:A:352:ALA:HB1	1:A:358:CYS:SG	2.55	0.47
1:A:378:ASP:OD1	1:A:379:ARG:CD	2.63	0.46
1:D:148:ILE:HG23	1:D:150:PHE:CE1	2.49	0.46
1:A:4:ILE:HG21	1:A:74:VAL:HG12	1.98	0.46
1:A:311:GLN:HE21	1:B:283:LEU:H	1.62	0.46
1:C:201:LYS:HG2	1:C:205:LEU:CD2	2.45	0.46
1:C:328:VAL:HG13	1:C:329:GLY:N	2.31	0.46
1:D:153:LEU:HD11	1:D:306:ARG:HD2	1.97	0.46
1:C:4:ILE:HG21	1:C:74:VAL:HG12	1.97	0.46
1:C:40:ARG:HG2	1:C:40:ARG:HH21	1.80	0.46
1:C:54:PHE:CB	1:C:357:LEU:HD21	2.44	0.46
1:C:105:GLU:HA	1:C:110:HIS:CG	2.50	0.46
1:A:190:THR:HG22	1:A:218:LYS:HE2	1.97	0.46
1:A:192:PRO:HB2	1:A:217:ILE:HD11	1.97	0.46
1:D:2:ARG:HG2	1:D:2:ARG:HH21	1.80	0.46
1:A:58:ARG:HH12	1:B:98:GLN:HG3	1.81	0.46
1:B:145:VAL:HG13	1:B:150:PHE:CE1	2.51	0.46
1:A:140:THR:OG1	1:A:143:GLN:HG3	2.16	0.46
1:A:182:GLU:HG3	1:A:183:GLN:HG3	1.98	0.46
1:B:392:LEU:HD22	1:B:413:GLU:CD	2.36	0.46
1:C:130:LYS:HB2	1:C:131:PRO:HD2	1.98	0.46
1:D:83:ILE:HG23	1:D:124:ALA:CB	2.46	0.46
1:A:221:VAL:HG22	1:A:247:VAL:HG13	1.98	0.45
1:B:145:VAL:HG21	1:B:163:LEU:HG	1.98	0.45
1:D:41:THR:OG1	1:D:47:LEU:HD12	2.16	0.45
1:A:58:ARG:HB2	1:B:98:GLN:HB2	1.97	0.45
1:A:157:LEU:HD22	1:A:340:LEU:HD13	1.99	0.45
1:A:201:LYS:O	1:A:205:LEU:HD13	2.17	0.45
1:B:350:PRO:HG2	1:B:365:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:GLY:O	1:B:354:GLY:C	2.54	0.45
1:C:145:VAL:HG13	1:C:150:PHE:CE1	2.52	0.45
1:C:190:THR:O	1:C:190:THR:HG22	2.17	0.45
1:C:282:VAL:HG22	1:C:312:LEU:HD13	1.97	0.45
1:B:133:TRP:H	1:B:363:HIS:CD2	2.28	0.45
1:B:190:THR:HG22	1:B:190:THR:O	2.16	0.45
1:B:217:ILE:HG12	1:B:218:LYS:N	2.32	0.45
1:C:55:THR:HG22	1:C:56:ILE:N	2.32	0.45
1:C:62:VAL:HG21	1:D:109:MET:HE2	1.96	0.45
1:D:433:ASP:O	1:D:435:ALA:N	2.49	0.45
1:C:308:VAL:O	1:C:312:LEU:HD22	2.16	0.45
1:B:239:ILE:HG23	1:B:243:ILE:CB	2.28	0.45
1:D:55:THR:HG22	1:D:57:GLY:H	1.82	0.45
1:C:221:VAL:HG22	1:C:247:VAL:HG13	1.99	0.45
1:D:13:ARG:CG	1:D:424:TYR:HB2	2.47	0.45
1:D:221:VAL:HB	1:D:228:ASP:OD1	2.17	0.45
1:A:311:GLN:HE22	1:B:282:VAL:N	2.14	0.45
1:B:387:LEU:N	1:B:387:LEU:CD1	2.80	0.45
1:D:191:SER:N	1:D:192:PRO:CD	2.79	0.45
1:D:199:ASP:OD2	1:D:230:ARG:NH2	2.50	0.45
1:A:424:TYR:CD1	1:A:425:PRO:HA	2.51	0.45
1:B:11:ASP:OD1	1:B:13:ARG:HD3	2.16	0.45
1:B:176:ARG:HD2	1:B:374:GLY:HA2	1.98	0.45
1:C:140:THR:O	1:C:144:LEU:HD23	2.17	0.45
1:A:153:LEU:HD11	1:A:306:ARG:HD2	1.98	0.44
1:A:176:ARG:HD2	1:A:370:VAL:HA	1.98	0.44
1:B:188:TYR:CB	1:B:216:THR:HB	2.47	0.44
1:C:104:PRO:HD3	1:D:302:HIS:CD2	2.52	0.44
1:A:123:LEU:HD23	1:A:123:LEU:O	2.17	0.44
1:C:93:LEU:HD22	1:C:93:LEU:N	2.32	0.44
1:A:386:HIS:HB3	1:A:387:LEU:CD2	2.47	0.44
1:B:41:THR:OG1	1:B:47:LEU:HD12	2.18	0.44
1:B:423:SER:O	1:B:427:GLY:HA3	2.17	0.44
1:A:106:LYS:NZ	1:B:304:GLN:HE21	2.16	0.44
1:A:135:PHE:O	1:A:139:LEU:HG	2.17	0.44
1:A:221:VAL:CG2	1:A:247:VAL:CG1	2.96	0.44
1:D:37:VAL:CG2	1:D:67:VAL:HG11	2.48	0.44
1:A:151:ARG:HD3	1:A:152:TYR:CZ	2.52	0.44
1:B:308:VAL:O	1:B:312:LEU:HD22	2.17	0.44
1:D:300:GLY:HA2	1:D:303:THR:OG1	2.18	0.44
1:A:83:ILE:HG13	1:A:124:ALA:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ASP:O	1:B:285:HIS:HD2	2.00	0.44
1:B:378:ASP:OD1	1:B:379:ARG:CD	2.66	0.43
1:C:188:TYR:CZ	1:C:382:GLU:HB2	2.53	0.43
1:C:193:GLY:HA3	1:C:219:LEU:HA	2.00	0.43
1:A:2:ARG:HG2	1:A:43:GLY:HA3	2.00	0.43
1:A:92:ARG:CB	1:A:92:ARG:HH21	2.31	0.43
1:B:44:ALA:O	1:B:47:LEU:N	2.48	0.43
1:C:221:VAL:HG21	1:C:247:VAL:CG1	2.48	0.43
1:C:428:ARG:HG2	1:C:428:ARG:NH1	2.31	0.43
1:D:229:ILE:HG13	1:D:268:PHE:CE1	2.53	0.43
1:B:180:LEU:HD23	1:B:180:LEU:C	2.38	0.43
1:D:271:ALA:O	1:D:272:TRP:HB3	2.19	0.43
1:D:322:GLN:HG3	1:D:349:PHE:O	2.19	0.43
1:A:97:SER:HB2	1:B:27:ASN:OD1	2.19	0.43
1:B:75:VAL:O	1:B:75:VAL:HG23	2.19	0.43
1:C:359:GLU:CD	1:C:395:VAL:HG13	2.39	0.43
1:D:170:GLN:HB3	1:D:171:PRO:HD3	1.99	0.43
1:A:200:GLU:CD	1:A:200:GLU:H	2.21	0.43
1:C:281:ASP:O	1:C:285:HIS:HD2	2.02	0.43
1:A:190:THR:HG22	1:A:218:LYS:HB3	2.01	0.43
1:A:419:ILE:N	1:A:419:ILE:HD12	2.33	0.43
1:B:148:ILE:HD11	1:B:150:PHE:CZ	2.53	0.43
1:D:392:LEU:HD22	1:D:413:GLU:CD	2.38	0.43
1:B:4:ILE:HG21	1:B:74:VAL:HG12	2.01	0.43
1:B:47:LEU:HD13	1:B:123:LEU:HD11	2.01	0.43
1:C:414:MET:CB	1:C:419:ILE:HD11	2.49	0.43
1:D:267:GLU:O	1:D:269:ASP:N	2.52	0.43
1:A:407:VAL:CG1	1:A:408:PRO:HD2	2.48	0.43
1:C:427:GLY:O	1:C:431:VAL:HG22	2.19	0.43
1:B:96:ASP:OD1	1:B:96:ASP:C	2.58	0.43
1:D:259:ILE:O	1:D:263:ARG:HG3	2.18	0.43
1:D:350:PRO:HG2	1:D:365:ALA:HB2	2.00	0.43
1:C:170:GLN:N	1:C:171:PRO:CD	2.82	0.42
1:A:39:LEU:HD11	1:A:74:VAL:HG11	1.99	0.42
1:A:189:THR:HG23	1:A:214:PHE:CD2	2.54	0.42
1:A:251:GLN:HE22	1:A:302:HIS:CD2	2.38	0.42
1:C:410:PHE:O	1:C:411:SER:HB2	2.19	0.42
1:B:47:LEU:CD1	1:B:123:LEU:HD11	2.48	0.42
1:C:201:LYS:O	1:C:205:LEU:HD23	2.19	0.42
1:C:391:PHE:O	1:C:394:PRO:HD3	2.19	0.42
1:D:2:ARG:HG2	1:D:2:ARG:NH2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:ASP:OD1	1:D:379:ARG:HD2	2.19	0.42
1:A:92:ARG:NH2	1:A:92:ARG:CB	2.83	0.42
1:D:308:VAL:O	1:D:312:LEU:HD22	2.19	0.42
1:A:8:GLU:HG2	1:A:38:VAL:HB	2.00	0.42
1:D:433:ASP:C	1:D:435:ALA:N	2.72	0.42
1:C:236:ARG:NH2	1:C:269:ASP:HB3	2.35	0.42
1:C:295:VAL:HA	1:C:296:PRO:HD3	1.88	0.42
1:A:167:ARG:O	1:A:170:GLN:HB3	2.20	0.42
1:B:43:GLY:O	1:B:45:GLU:N	2.52	0.42
1:C:3:THR:HG23	1:C:77:LEU:O	2.19	0.42
1:A:282:VAL:HG22	1:A:312:LEU:HD13	2.02	0.42
1:A:304:GLN:HE21	1:B:106:LYS:NZ	2.17	0.42
1:C:150:PHE:CZ	1:C:159:ARG:HA	2.55	0.42
1:D:55:THR:CG2	1:D:56:ILE:N	2.82	0.42
1:D:176:ARG:CD	1:D:374:GLY:HA2	2.49	0.42
1:D:253:TRP:HB2	1:D:258:ALA:HB2	2.01	0.42
1:C:26:MET:HE1	3:D:621:HOH:O	2.20	0.42
1:D:44:ALA:C	1:D:46:ASP:H	2.21	0.42
1:A:71:ALA:O	1:A:75:VAL:HG22	2.20	0.41
1:B:142:GLU:CG	1:D:200:GLU:HG2	2.48	0.41
1:B:210:VAL:CG2	1:B:239:ILE:HG13	2.50	0.41
1:C:62:VAL:HG21	1:D:109:MET:HE1	2.01	0.41
1:C:304:GLN:HE21	1:C:304:GLN:HB3	1.70	0.41
1:C:305:ASN:HB2	1:C:333:GLU:OE1	2.20	0.41
1:B:55:THR:CG2	1:B:56:ILE:N	2.82	0.41
1:C:414:MET:HB2	1:C:419:ILE:HD11	2.02	0.41
1:D:44:ALA:C	1:D:46:ASP:N	2.73	0.41
1:D:309:PHE:CE1	1:D:337:ILE:HD13	2.55	0.41
1:B:13:ARG:CG	1:B:424:TYR:HB2	2.51	0.41
1:C:324:ASP:OD2	1:C:351:HIS:HD2	2.03	0.41
1:D:75:VAL:HG23	1:D:75:VAL:O	2.19	0.41
1:B:159:ARG:HG2	1:B:159:ARG:HH11	1.85	0.41
1:B:303:THR:HB	1:B:309:PHE:CE1	2.55	0.41
1:B:308:VAL:HG12	1:B:312:LEU:CD2	2.50	0.41
1:D:102:LEU:N	1:D:102:LEU:HD22	2.34	0.41
1:A:29:ASP:N	1:A:30:PRO:HD3	2.35	0.41
1:A:73:HIS:HE1	1:A:96:ASP:OD2	2.03	0.41
1:B:221:VAL:HG21	1:B:247:VAL:HG11	2.02	0.41
1:C:139:LEU:HD12	1:C:144:LEU:HD13	2.03	0.41
1:C:239:ILE:HG23	1:C:243:ILE:CB	2.32	0.41
1:C:350:PRO:HG2	1:C:365:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ILE:HG13	1:A:124:ALA:HB2	2.02	0.41
1:C:44:ALA:C	1:C:46:ASP:N	2.73	0.41
1:C:387:LEU:HD22	1:C:387:LEU:N	2.35	0.41
1:C:419:ILE:HD12	1:C:419:ILE:N	2.36	0.41
1:B:99:LEU:HD12	1:B:99:LEU:HA	1.91	0.41
1:C:282:VAL:N	1:D:311:GLN:NE2	2.67	0.41
1:C:323:ILE:HD11	1:C:337:ILE:HG22	2.02	0.41
1:D:255:VAL:O	1:D:259:ILE:HG13	2.21	0.41
1:D:281:ASP:O	1:D:285:HIS:HD2	2.04	0.41
1:A:9:THR:HB	1:A:64:THR:HG23	2.03	0.41
1:A:52:LEU:HD12	1:A:52:LEU:O	2.21	0.41
1:A:144:LEU:HD12	1:A:144:LEU:HA	1.97	0.41
1:A:148:ILE:HD12	1:A:149:ASP:N	2.36	0.41
1:A:188:TYR:CZ	1:A:382:GLU:HB2	2.56	0.41
1:A:230:ARG:HH21	1:A:230:ARG:HG2	1.86	0.41
1:A:271:ALA:O	1:A:272:TRP:HB3	2.21	0.41
1:B:55:THR:HG21	1:B:60:ASN:CB	2.50	0.41
1:B:134:ARG:O	1:B:138:GLU:HG3	2.21	0.41
1:C:52:LEU:N	1:C:52:LEU:CD2	2.84	0.41
1:C:192:PRO:HG3	1:C:217:ILE:HD11	2.02	0.41
1:C:262:MET:HE2	1:C:265:LEU:HD12	2.01	0.41
1:C:368:ASP:OD2	1:C:373:THR:HG23	2.20	0.41
1:C:434:LEU:N	1:C:434:LEU:HD22	2.36	0.41
1:A:47:LEU:HD22	1:A:47:LEU:HA	1.86	0.41
1:B:3:THR:CG2	1:B:4:ILE:N	2.84	0.40
1:C:305:ASN:HA	1:C:328:VAL:HG23	2.03	0.40
1:A:2:ARG:HG2	1:A:43:GLY:CA	2.51	0.40
1:B:396:ARG:HH11	1:B:396:ARG:CG	2.33	0.40
1:C:219:LEU:HD11	1:C:235:ALA:CB	2.51	0.40
1:D:25:ALA:N	1:D:195:LEU:HD12	2.36	0.40
1:A:384:VAL:CG1	1:A:386:HIS:ND1	2.85	0.40
1:B:3:THR:HG22	1:B:4:ILE:N	2.37	0.40
1:B:55:THR:HB	1:B:60:ASN:OD1	2.22	0.40
1:B:300:GLY:HA2	1:B:303:THR:OG1	2.22	0.40
1:D:47:LEU:CD1	1:D:123:LEU:HD21	2.46	0.40
1:D:356:GLY:HA2	1:D:359:GLU:OE2	2.22	0.40
1:D:378:ASP:OD1	1:D:379:ARG:HD3	2.21	0.40
1:A:185:TYR:CD1	1:A:186:PRO:HD2	2.57	0.40
1:A:218:LYS:HA	1:A:246:ALA:O	2.22	0.40
1:C:53:VAL:CG2	1:C:115:ALA:HB2	2.51	0.40
1:C:407:VAL:CG1	1:C:408:PRO:HD2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:LYS:CG	1:D:238:ALA:HB1	2.50	0.40
1:D:387:LEU:HD12	1:D:387:LEU:H	1.85	0.40
1:A:8:GLU:HG3	1:A:38:VAL:HB	2.01	0.40
1:A:28:PRO:O	1:A:30:PRO:HD3	2.20	0.40
1:A:47:LEU:HD13	1:A:47:LEU:C	2.42	0.40
1:B:102:LEU:HD12	1:B:109:MET:CE	2.51	0.40
1:C:104:PRO:O	1:C:106:LYS:HE3	2.21	0.40
1:C:306:ARG:HH11	1:C:306:ARG:HG2	1.86	0.40
1:D:2:ARG:HG2	1:D:2:ARG:H	1.49	0.40
1:D:220:LYS:NZ	3:D:668:HOH:O	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	422/436 (97%)	405 (96%)	17 (4%)	0	100	100
1	B	430/436 (99%)	412 (96%)	16 (4%)	2 (0%)	29	23
1	C	432/436 (99%)	405 (94%)	25 (6%)	2 (0%)	29	23
1	D	429/436 (98%)	407 (95%)	19 (4%)	3 (1%)	22	16
All	All	1713/1744 (98%)	1629 (95%)	77 (4%)	7 (0%)	34	30

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	44	ALA
1	D	268	PHE
1	D	434	LEU
1	D	269	ASP
1	C	22	GLY

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Mol	Chain	Res	Type
1	C	387	LEU
1	B	328	VAL

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	334/340 (98%)	314 (94%)	20 (6%)	19	14
1	B	338/340 (99%)	325 (96%)	13 (4%)	33	31
1	C	340/340 (100%)	321 (94%)	19 (6%)	21	17
1	D	338/340 (99%)	316 (94%)	22 (6%)	17	12
All	All	1350/1360 (99%)	1276 (94%)	74 (6%)	21	17

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	31	ASP
1	A	47	LEU
1	A	86	LEU
1	A	93	LEU
1	A	99	LEU
1	A	148	ILE
1	A	151	ARG
1	A	172	GLN
1	A	180	LEU
1	A	200	GLU
1	A	239	ILE
1	A	302	HIS
1	A	312	LEU
1	A	340	LEU
1	A	357	LEU
1	A	361	VAL
1	A	377	GLU
1	A	379	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	410	PHE
1	B	13	ARG
1	B	39	LEU
1	B	52	LEU
1	B	99	LEU
1	B	126	ARG
1	B	148	ILE
1	B	172	GLN
1	B	202	LEU
1	B	313	LEU
1	B	361	VAL
1	B	379	ARG
1	B	396	ARG
1	B	410	PHE
1	C	13	ARG
1	C	39	LEU
1	C	52	LEU
1	C	99	LEU
1	C	123	LEU
1	C	129	ASN
1	C	148	ILE
1	C	159	ARG
1	C	172	GLN
1	C	195	LEU
1	C	273	ILE
1	C	302	HIS
1	C	304	GLN
1	C	312	LEU
1	C	313	LEU
1	C	323	ILE
1	C	340	LEU
1	C	379	ARG
1	C	410	PHE
1	D	13	ARG
1	D	39	LEU
1	D	52	LEU
1	D	80	ASP
1	D	93	LEU
1	D	123	LEU
1	D	144	LEU
1	D	148	ILE
1	D	159	ARG

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Mol	Chain	Res	Type
1	D	172	GLN
1	D	180	LEU
1	D	239	ILE
1	D	273	ILE
1	D	293	THR
1	D	302	HIS
1	D	313	LEU
1	D	340	LEU
1	D	357	LEU
1	D	361	VAL
1	D	379	ARG
1	D	410	PHE
1	D	425	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	73	HIS
1	A	285	HIS
1	A	302	HIS
1	A	304	GLN
1	A	311	GLN
1	A	314	GLN
1	A	351	HIS
1	A	363	HIS
1	A	390	HIS
1	B	63	GLN
1	B	73	HIS
1	B	170	GLN
1	B	172	GLN
1	B	183	GLN
1	B	250	ASN
1	B	285	HIS
1	B	304	GLN
1	B	311	GLN
1	B	314	GLN
1	B	351	HIS
1	B	363	HIS
1	B	390	HIS
1	C	73	HIS
1	C	95	ASN

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Mol	Chain	Res	Type
1	C	170	GLN
1	C	172	GLN
1	C	226	GLN
1	C	250	ASN
1	C	285	HIS
1	C	302	HIS
1	C	304	GLN
1	C	311	GLN
1	C	314	GLN
1	C	351	HIS
1	C	363	HIS
1	C	389	GLN
1	C	390	HIS
1	D	63	GLN
1	D	73	HIS
1	D	170	GLN
1	D	172	GLN
1	D	183	GLN
1	D	250	ASN
1	D	285	HIS
1	D	302	HIS
1	D	304	GLN
1	D	311	GLN
1	D	314	GLN
1	D	351	HIS
1	D	363	HIS
1	D	390	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	426/436 (97%)	0.00	13 (3%) 49 48	21, 34, 58, 84	0
1	B	432/436 (99%)	-0.07	8 (1%) 66 65	21, 32, 55, 87	0
1	C	434/436 (99%)	0.17	15 (3%) 44 43	21, 39, 68, 88	0
1	D	433/436 (99%)	0.10	18 (4%) 36 35	24, 36, 59, 84	0
All	All	1725/1744 (98%)	0.05	54 (3%) 49 48	21, 35, 60, 88	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	46	ASP	7.7
1	A	434	LEU	5.7
1	D	234	LEU	5.3
1	C	46	ASP	4.8
1	C	432	GLU	4.7
1	C	45	GLU	4.5
1	D	202	LEU	4.3
1	A	28	PRO	4.2
1	B	43	GLY	4.2
1	D	235	ALA	4.1
1	D	196	GLY	4.1
1	C	434	LEU	4.1
1	B	46	ASP	3.9
1	D	199	ASP	3.7
1	A	47	LEU	3.7
1	A	45	GLU	3.5
1	C	431	VAL	3.4
1	B	47	LEU	3.3
1	D	434	LEU	3.3
1	B	431	VAL	3.2
1	D	237	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	425	PRO	3.2
1	D	1	MET	3.1
1	B	426	ASP	3.1
1	D	436	ALA	3.1
1	C	47	LEU	3.0
1	A	424	TYR	2.9
1	A	432	GLU	2.9
1	D	238	ALA	2.8
1	A	29	ASP	2.8
1	B	1	MET	2.7
1	D	239	ILE	2.7
1	C	20	LEU	2.6
1	A	102	LEU	2.6
1	A	18	ARG	2.5
1	C	21	ASP	2.5
1	A	103	GLY	2.5
1	B	45	GLU	2.5
1	D	205	LEU	2.4
1	C	43	GLY	2.4
1	B	427	GLY	2.4
1	C	357	LEU	2.4
1	A	426	ASP	2.4
1	C	428	ARG	2.3
1	D	204	ARG	2.2
1	C	422	PHE	2.2
1	D	46	ASP	2.2
1	A	428	ARG	2.1
1	C	328	VAL	2.1
1	D	2	ARG	2.1
1	C	18	ARG	2.0
1	D	323	ILE	2.0
1	D	200	GLU	2.0
1	D	203	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	D	604	1/1	0.78	0.26	56,56,56,56	0
2	MG	C	603	1/1	0.83	0.18	37,37,37,37	0
2	MG	B	602	1/1	0.91	0.16	31,31,31,31	0
2	MG	A	601	1/1	0.97	0.10	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.